Possible phase-sensitive tests of pairing symmetry in pnictide superconductors

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The discovery of the new class of pnictide superconductors has engendered a controversy about their pairing symmetry, with proposals ranging from an extended s-wave or "$s_\pm$" symmetry to nodal or nodeless d-wave symmetry to still more exotic order parameters such as p-wave. In this paper, building on the earlier, similar work performed for the cuprates, we propose several phase-sensitive Josephson interferometry experiments, each of which may allow resolution of the issue.

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Identification of order parameter symmetry is one of the first tasks the condensed matter physics community faces upon discovery of a new superconductor. Historically, as pointed out by Harlingen [1], methods of determining order parameter symmetry have fallen into two classes: techniques which are sensitive to the *magnitude* of the order parameter, and techniques which are sensitive to the *phase*. Most of the magnitude sensitive techniques are ultimately concerned with the presence of Fermi surface nodes. Examples include thermodynamic tests such as density-of-states, specific heat, and London penetration depth. The first experimental technique to yield detailed information about the momentum dependence of the order parameter was angle-resolved photoemission spectroscopy (for a review, see Ref. [2]), or ARPES, which demonstrated the substantial momentum anisotropy in the high-temperature cuprate gap function.

None of these tests, however, is a "smoking gun" ultimately capable of unequivocally determining the order parameter structure. For this one also requires a phase-sensitive test, such as the Josephson interferometry [3] or tricrystal junctions [4]. Such tests, as originally proposed by Geshkenbein et al [5], Rice and Sigrist [6], and Leggett [3] provided highly convincing evidence for d-wave superconductivity in the cuprates, effectively ending a controversy of several years, and have been also used to address p-wave superconductivity in Sr_2RuO_4[7].

We now consider such a test of order parameter symmetry in the pnictide superconductors, which have been extensively investigated since the original discovery by Kamihara early in 2008 [8]. There are now dozens of superconductors in this family, with superconducting transition temperatures T_c as high as 57 K. Bandstructure calculations and ARPES data indicate that these materials contain disjoint Fermi surfaces, as illustrated in Figure 1, with a hole pocket centered around (0,0) and electron pockets at (π,π) and related points.

Despite this effort, the gap symmetry of the pnictides remains unknown. A potential pnictide gap function presently receiving much consideration is the "$s_\pm$" state [9], in which the order parameter changes sign from the hole to electron Fermi surfaces, but is roughly constant on each Fermi surface, with no nodes.

To date, there have been three phase-sensitive experiments performed on the pnictides. The first is the observation in inelastic neutron scattering (INS) measurements on $Ba_{0.6}K_{0.4}Fe_2As_2$[10] of a resonance peak centered at $\mathbf{Q} = (\pi,\pi)$ that appears below T_c. This effect has been well-studied in connection to the cuprates [11], and in pnictides it had been predicted theoretically for the $s_\pm$ states because of the change in order parameter sign [9, 12, 13] over the vector $\mathbf{Q}$. More recently, an ab-corner junction experiment was performed [14] on $BaFe_{1.8}Co_{0.2}As_2$, which found no evidence for a phase shift between the a and b directions, suggesting that the d-wave symmetry observed in the cuprates is not present in this material. Similarly, Zhang et al [15] fabricated c-axis Josephson junctions between a conventional superconductor and $Ba_{1-x}K_xFe_2As_2$ and observed Josephson coupling, suggestive of an s-wave state, but not providing clear evidence for the $s_\pm$ state itself.

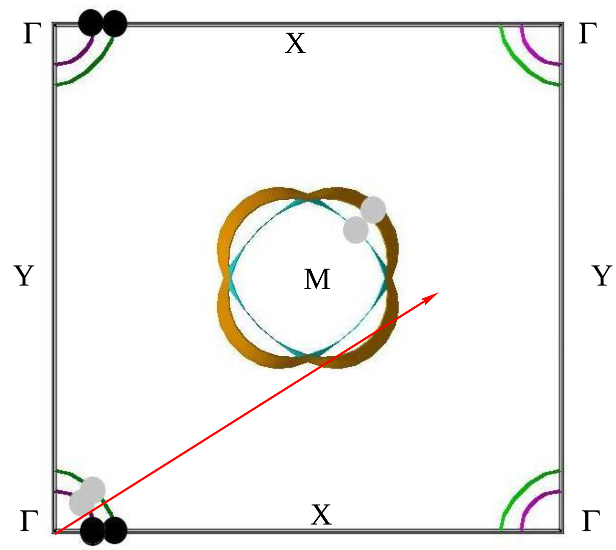

FIG. 1: (Color online) A view of the calculated Fermi surface geometry in a superconducting pnictide $LaFeAsO_{0.9}F_{0.1}$, with hole (Γ) and electron pockets (M) indicated. For a thick barrier the black circles represent the Fermi surface states which dominate the (100) current, while the grey circles represent the states which dominate the (110) current. A possible intermediate angle, where the electron surface may dominate the current, is shown by the arrow.

In this paper we propose direct phase-sensitive tests, based upon Josephson interferometry, that could provide strong evidence for an $s_\pm$ state, if existent. The proposal is based on an adaptation of the famous "corner junction" experiments performed for the cuprates.

We briefly review the theory of corner junctions and their application to the cuprates and Sr_2RuO_4. In a corner junction, the Josephson current is allowed to flow from two separate faces of a single crystal of unconventional superconductor. A junction usually preferentially samples current oriented along the normal to the interface. By measuring the critical current flow as a function of magnetic field, one can determine the phase difference between the two directions sampled. Such experiments were enormously successful in determining the pairing symmetry in the high-temperature cuprates [3], and have been also applied to Sr_2RuO_4.[7]

One key to these experiments has been the existence of symmetry constraints dictating a particular phase difference for specific crystallographic directions. In d-wave superconductors, the phase must change by π upon a 90^o rotation, while in p-wave materials upon a 180^o rotation. For the $s_\pm$ state with two or more disconnected Fermi surfaces, as in the pnictides, the situation becomes much more complicated. The familiar from cuprates a/b-plane corner junction will not find phase differences since the a and b directions are equivalent for the $s_\pm$ state. On the other hand, a/c junctions may work, if the in-plane and the out-of-plane transport are dominated by different bands. In the simplest approximation for a specular (infinitely thin) barrier this amounts to comparing the number of conductivity channels for each direction, given by the DOS-weighted average of the corresponding Fermi velocity, *e.g.*, $n_z = \langle N(E_F)v_{Fz}\rangle$[17].

Unfortunately, in the e-doped 1111 compounds, transport in both a and c directions is dominated by the e-pocket [9] (cf. Figure 1). A glance at the Fermi surface of a hole-doped 112 material (Figure 4, dark red) shows that here again the transport in all directions is dominated by the same band, this time the hole one. Thus, phase-sensitive experiments do not at first appear to be feasible for detecting an $s_\pm$ state in the pnictides.

There is, however, one additional degree of freedom which may help design a phase-sensitive experiment. For a specular barrier, all wavevectors from all Fermi surfaces contribute to the current, regardless of tunneling direction (that is, of $k_\parallel$). However, for a barrier of an appreciable thickness, this is not the case. The general expression for the Josephson current between two superconductors is well-known and we repeat it here:

$$J \propto \langle T_{\mathbf{k}} Im[\Delta_s^* \Delta_0(\mathbf{k})]\rangle$$

Here Δ_s is the gap on the conventional superconductor and $\Delta_0(\mathbf{k})$ the gap on the pnictide, and the $\langle ...\rangle$ means an average over the states on the pnictide Fermi surface whose Fermi velocity contains a positive projection on the tunneling direction, which is perpendicular to the sample interface. The $T_{\mathbf{k}}$ is the tunneling probability, which for a thick barrier decreases exponentially with $k_\parallel$[16]. For instance, for a thick vacuum barrier the transparency is

$$T_{\mathbf{k}} = \frac{4m_0^2\hbar^2K^2v_Lv_R}{\hbar^2m_0^2K^2(v_L+v_R)^2+(\hbar^2K^2+m_0^2v_L^2)(\hbar^2K^2+m_0^2v_R^2)\sinh^2(dK)} \quad (1)$$

Here m_0 is the electron mass, $v_{L,R}$ are the Fermi velocity projections the tunneling directions, d is the width of the barrier, and the quasimomentum of the evanescent wavefunction in the barrier, iK, is, from energy conservation,

$$K = \sqrt{k_\parallel^2 + 2(U-E)m_0},$$

where U is the barrier height.

Now we observe that for an interface normal in the (100) direction, the electron Fermi surfaces have a huge $k_\parallel$ of approximately π/a, with a the lattice constant, and will be exponentially suppressed for a barrier of any appreciable thickness. The same is not true for the Γ centered hole Fermi surfaces, $k_\parallel \ll \pi/a$. Note that a thick barrier need not have very low transparency: the transparency is defined by both height (which may be low) and thickness, while the filtering properties are defined by the thickness only. So, for a thick low barrier we will have Josephson current dominated by the hole states in the (100) direction, while for the (110) direction both holes and electrons will contribute. Unlike for the specular barrier, we cannot now determine which band will dominate the (110) current, because the geometric factor becomes irrelevant, as long as there are states with $k_\parallel = 0$ (cf. Fig. 1). A combination of the Fermi velocity and the wave function at the "hot spot" determines the current[16], and needs to be estimated for each superconductor and for each barrier material. For instance, in LaFeAsO and a vacuum barrier it appears that the hole pocket (mostly xz/yz symmetry, that cannot tunnel into vacuum) has a considerable admixture of the z^2 symmetry and thus will have a higher tunneling matrix element than the electron pocket, mostly of the x^2-y^2, xz, and yz symmetry, none of which can tunnel along (110). Numerical estimates, based on the first principle calculations, show that the current from the e-pocket is maximized at an intermediate angle as shown in Fig. 1. It is hard to estimate with confidence, though, whether at this angle it will overcome the hole current, as needed for a detectable corner-junction phase shift.

While it may be worth trying to search experimentally for a π-shift in a (100)-$(\cos\alpha, \sin\alpha, 0)$ geometry, one can think of a more promising design. Indeed, let us consider a corner-junction experiment where the (100) junction is a thick-barrier contact (which as we just discussed, is dominated by the h-pockets), and the second contact is a (010) or a (001) *specular*-barrier junction. As discussed in the beginning, either of these last contacts in an electron-doped material will be dominated by the e-pockets, thus providing the desired π shift. A possible geometry is illustrated in Figure 2, if the $s_\pm$ state is present.

The basic point here is that, unlike in the cuprates and Sr_2RuO_4, directional selection is not sufficient to select the appropriate region of Fermi surface to sample to uncover a π

phase shift. One must use additional selection means, in this case given by the use of different barrier characteristics in different directions.

Regarding the width and height of the non-specular potential barrier, the key consideration is that the electron FS be suppressed greatly without a comparable suppression of the hole FS. For a moderate barrier height $U-E=0.25$ eV (which would require a barrier made out of a small-gap semiconductor, $E_g \sim 0.5$ eV) a barrier of width 20 Å would only suppress the hole-like Fermi surface by roughly a factor of 9 ($\sinh^2 1.8$), while suppressing the electron Fermi surface by a factor of $\sinh^2 20 \sim 10^{16}$. The calculated hole-like surface suppression factor neglects the effect of a small but finite range in $k_{\|}$ for this Fermi surface, whose inclusion could result in a somewhat larger suppression. We also implicitly assume a substantially electron-doped pnictide, so that specular transport is governed uniquely by the electron Fermi surface.

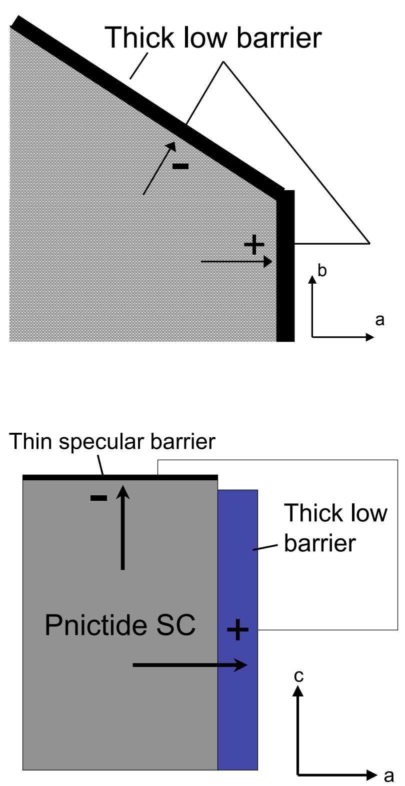

FIG. 2: A schematic view of tunneling geometry for two possible experiments: top, a (100) -near-(110) orientation, bottom, an ac orientation with specular and thick barriers as indicated.

A possible disadvantage of the proposed experiment is that it requires a rather fine control over the interface properties. However, there is yet another possibility of designing a two-junction experiment with a π shift. This requires, however, a *bi*crystal as shown in Fig. 3. We propose to grow epitaxially a bicrystal of a hole-doped ($Ba_{1-x}K_xFe_2As_2$) and an electron-doped ($BaFe_{2(1-x)}Co_{2x}As_2$) materials. As discussed above, the doping enhances the size and Fermi velocity of the respective Fermi surfaces, and the conductance is dominated by the hole or electron Fermi surface, correspondingly. The only remaining problem is to ensure the proper phase coherence, that is, that the holes in both crystals have the same phase, and the electrons the same, but opposite to that of the holes.

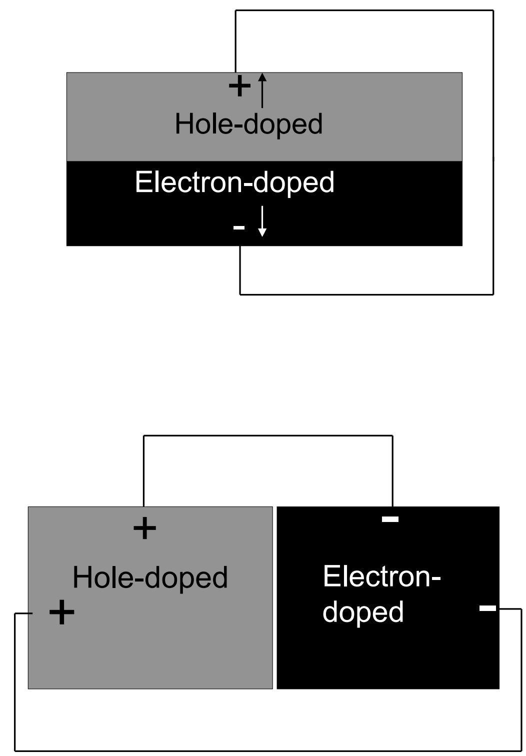

FIG. 3: A schematic view of the tunneling geometry for the proposed bicrystal experiments. Top: a c-axis orientation; bottom, an ab-plane orientation with two possible lead orientations.

In case of an epitaxial (coherent) interface the parallel wave vector, $k_{\|}$, is conserved through the interface, and the way to ensure that the h-h and e-e currents are much larger than the e-h and h-e current is to ensure that the overlap of the FS projections onto the interface plane is maximal for the e-e and h-h overlaps, as opposed to the e-h overlap. Obviously, this condition is satisfied in a bicrystal with a (100) interface – there is no e-h overlap at all, and the e-e and h-h overlaps are nearly maximal possible. Unfortunately, growing an epitaxial (100) interface may be very difficult.

On the other hand, growing a (001), or “c-axis” interface is much more natural. Let us consider the FS overlaps in this case. Figure 4 plots the projections of the calculated[18] Fermi surfaces of $BaFe_{1.6}Co_{0.4}As_2$ (dark red) and $Ba_{0.6}K_{0.4}Fe_2As_2$ (light green). In this figure the three dimensional Fermi surfaces have been telescoped onto the basal plane, so that what one sees is the extent of the Fermi surface in the planar direction across all wavevectors. The doping levels of $\pm 20\%$ were chosen because this is the "critical" spread at which the direct overlap of the e-FSs nearly disappears. At any smaller spread there is either direct e-e overlap or both e-e and h-h overlaps. Obviously, there is no e-h overlap and e-h transport requires substantial nonconservation of the parallel momentum.

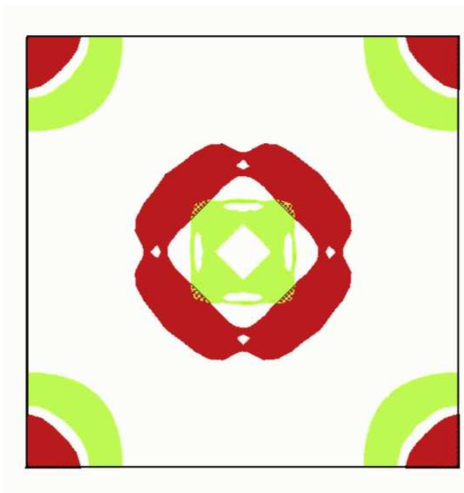

FIG. 4: (Color online) A first-principles calculation of the ab-plane projected three dimensional Fermi surfaces of $Ba_{0.6}K_{0.4}Fe_2As_2$ (green/gray) and $BaFe_{1.6}Co_{0.4}As_2$ (red/black).

In conclusion, we have proposed several phase-sensitive Josephson tests of the ostensible $s_{\pm}$ order parameter symmetry in the superconducting pnictides. The first design involves ab-plane corner junctions with angles smaller than 90^0, the second either ab or ac 90^0 junctions, prepared in such a way that one junction barrier is thin (specular) and the other thick, and the third, probably the most promising one, uses epitaxially grown hole- and electron-doped bicrystals in a "sandwich" orientation. We await the results of such Josephson tunneling experiments with great interest.

It must be pointed out that there are several unknowns complicating observation of the interferometric effect proposed. As opposed to d- or p-wave pairing, the π shift here is not a qualitative, symmetry determined effect, but a quantitative one, based upon favorable relations for tunneling probabilities for different bands. While we have taken into account some major factors, accurate calculations of the said probabilities are not possible. Interface properies may greatly affect them.

For these reasons the arguments given above should be considered in the following light: if a π phase shift between the electron and hole Fermi surfaces is observed in any of the prposed geometries, this would be extremely strong evidence for an $s_{\pm}$ state; unfortunately, the lack of observation of such a shift in any given experiment cannot be taken as similarly strong evidence against such a state.

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[1] D.J. van Harlingen, Rev. Mod. Phys. 67, 515 (1995).
[2] A. Damascelli, Z. Hussain, and Z.X. Shen, Rev. Mod. Phys. 75, 473 (2003).
[3] D.A. Wollman, D.J. van Harlingen, W.C. Lee, D.M. Ginsberg, and A.J. Leggett, Phys. Rev. Lett. 71, 2134 (1994).
[4] C.C. Tsuei et al, Phys. Rev. Lett. 73, 593 (1994).
[5] V.B. Geshkenbein, A.I. Larkin and A. Barone, Phys. Rev. B 36, 235 (1987).
[6] M. Sigrist and T.M. Rice, J. Phys. Soc. Jpn. 61, 4283 (1992).
[7] K.D. Nelson et al., Science 306, 1142 (2004).
[8] Y. Kamihara et al, J. Am. Chem. Soc. 130, 3296 (2008).
[9] I.I. Mazin, D.J. Singh, M.D. Johannes and M.H. Du, Phys. Rev. Lett. 101, 057003 (2008).
[10] A.D. Christianson et al, arXiv:0807.3932.
[11] E. Demler, W. Hanke and S.C. Zhang, Rev. Mod. Phys. 76, 909 (2004).
[12] M. M. Korshunov and I. Eremin, Phys. Rev. B 78, 140509(R), (2008).
[13] T.A. Maier and D.J. Scalapino, Phys. Rev. B **78**, 020514 (2008).
[14] Y.-R. Zhou et al, arXiv:0812.3295.
[15] X. Zhang et al, arXiv:0812.3605.
[16] I.I. Mazin, Europhys. Lett. 55, 3 (2001).
[17] I.I. Mazin, Phys. Rev. Lett., 83, 1427 (1999).
[18] We used the linear augmented plane wave method (LAPW) in the virtual crystal approximation, as discussed in Ref. [9].